FLOW AND REACTION SIMULATION OF A TUNGSTEN CVD REACTOR

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To minimize and understand the variability of a CVD process, it is necessary to investigate effect of the temperature, flow, pressure, and reaction kinetics in the reactor. Process simulation provides a fast and cost effective alternative because it identifies the physical and chemical environment at the wafer surface and allows the optimization for higher deposition rates, and better uniformity. In addition, it provides visual feedback in space and time on the variables that control the reaction and the effect that equipment settings have on deposition rate *[1, 2]*. This work presents the two dimensional flow, temperature, pressure, and kinetic simulation of a cold wall tungsten CVD reactor with models that determine the selectivity to oxide from the concentration of hydrogen fluoride (HF) at the wafer surface *[3]*.

The simulations are based on the computation of the Navier-Stokes, mass continuity, and heat transfer equations using the program PHOENICS *[4]* with some changes to include surface reaction kinetics and boundary conditions. The reactor is incorporated in 2 and 3 dimensional simulations in cylindrical coordinates taking advantage of the symmetry of the problem. The reaction kinetics are based on the thermal decomposition of tungsten hexafluoride (WF_6) by hydrogen (H_2) through the reaction

$$WF_6(g) + 3\,H_2(g) \text{ -------> } W(s) + 6\,HF(g)$$

with a deposition rate R_w described by a mass transfer R_d and reaction kinetics R_k limited regions by the equation

$$1/R_w = 1/R_d + 1/R_k$$

The mass transfer is determined by a diffusive flux (J_d) in the boundary layer (X_l) assuming the concentration of WF_6 is zero at the wafer surface

$$R_d = J_d/d_w = 1/d_w\, D_{wf6}\, N_w(X_l)/X_l$$

where d_w is the density of cvd tungsten, D_{wf6} is an estimation of the diffusion coefficient of WF_6 in H_2 *[5]* at the operating conditions, and N_w is the concentration of WF_6 at the sheath boundary. The kinetics limited regime is described by an Arrhenius equation proportional to the square root of the partial pressure of H_2 *[6, 7]* as

$$R_k = k_o \exp(-E_a/k_T)\, P_{H2}^{1/2}$$

where $k_o = 4.08 \times 10^6$ (nm min^{-1} $Pa^{-1/2}$); the activation energy $E_a = 0.75$ eV. From the deposition rate, the consumption of WF_6 and the generation of HF are computed as a function of position along the wafer. These equations are solved self consistently to derive the partial pressures of WF_6, H_2, and HF and the deposition rate in the reactor. The effects of viscosity as a function of temperature and composition are included in the results. A simple heat conduction model was incorporated to account for the temperature difference between the temperature measured at the holder and the temperature at the wafer. This temperature difference was typically of the order of 50 - 70 K.

The boundary conditions for flow and temperature are the ones found in the cold wall reactor where the wafer faces down and is heated by halogen lamps. The gas mixture is introduced at the bottom and is heated by conduction from the wafer. The range of conditions used in the simulation are for pressure (100 - 900 mT), temperature 650 - 850 K, and flows 100 - 2000 sccm of H_2, and 0 - 50 sccm of WF_6.

From the results of Fig. 1, the flow was found to be laminar even at 2000 sccm total flow, which is explained by small Reynolds number in the system ($Re < 1$). The temperature increases from the gas inlet to the wafer and is reduced near the pumping port. Figure 2 and 3 illustrate typical concentration of WF_6 and HF near the wafer surface using a non-reactive holder. The concentration of WF_6 on the wafer is reduced slightly and does not bring the reaction into mass transport limited regime. In the simulation conditions, the diffusion flux is larger than the convective flux making the HF concentration somewhat independent of flow; however, if there is a large source of HF near the wafer, there is a direct increase in concentration at the center.

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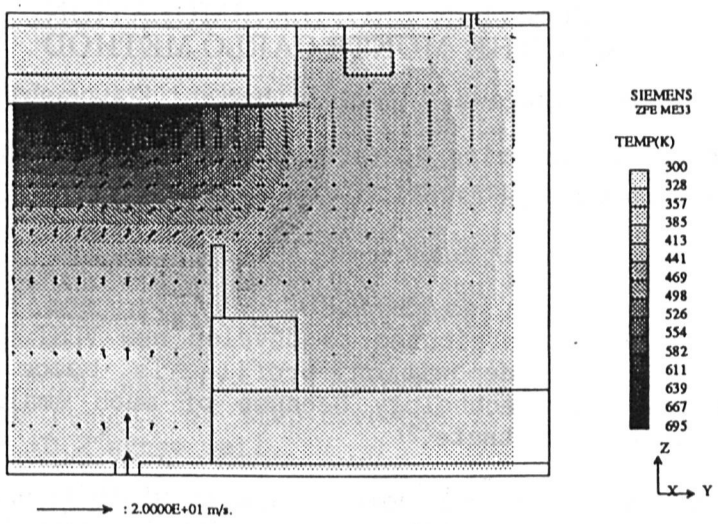

Fig. 1) Temperature and flow contours inside the CVD reactor. The flow is laminar and the temperature increases as the gas approaches the hot wafer.

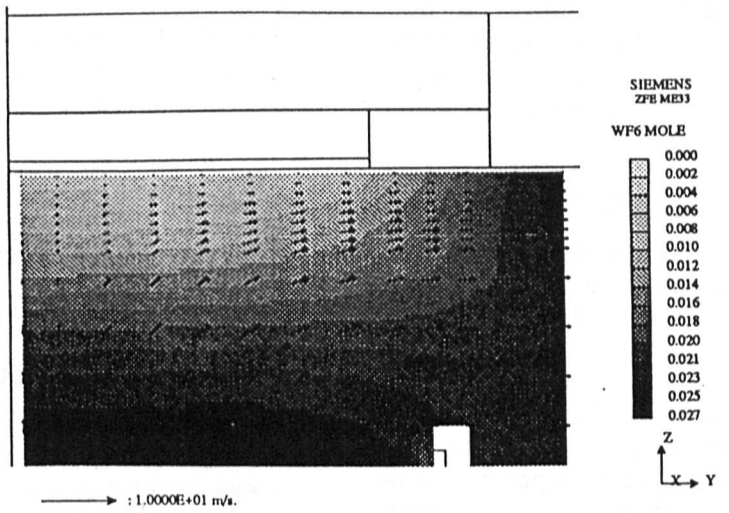

Fig. 2) Concentration contours of tungsten hexafluoride near the wafer.

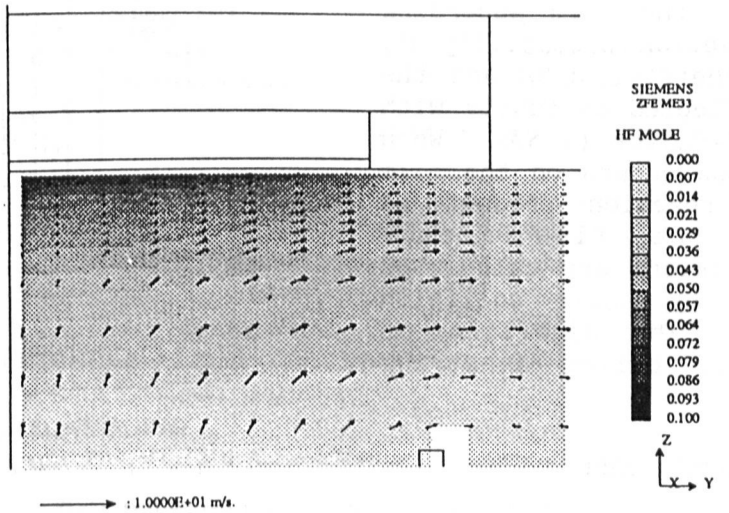

Fig. 3) Concentration contours of hydrogen fluoride near the wafer.